ERSP PI Meeting Breakout Session:
Summary Report on Identifying New Science Opportunities for DOE Sites

John Zachara (PNNL) and Eric Roden (University of Wisconsin)

Tuesday, April 4, 2006

The Environmental Remediation Science Program (ERSP) was established in FY 06 by merging the previous NABIR and EMSP Programs. Coincident with this programmatic change, the Environmental Remediation Sciences Division (ERSD) has revised their strategic plan http://www.science.doe.gov/ober/ERSD_top.html to define the future goals and directions of the new ERSP program. A breakout session was held at the first annual ERSP program meeting to identify and discuss new science themes for the ERSP that extend past NABIR and EMSP research activities on the reductive immobilization of uranium and other polyvalent radionuclides and metals to less explored, but equally relevant and important scientific issues (see Abstract, **Attachment I**). The breakout session specifically sought input from meeting participants on new science questions, issues, and opportunities in fate and transport, and remediation science research for DOE lands. Because of ERSD's programmatic focus on environmental microbiology, the breakout session placed emphasis on research related to the coupling of microbiologic, hydrologic, and geochemical processes. However, many participants stated that critical disciplinary issues in microbiology, hydrology, and geochemistry need to be resolved before more complex, coupled process studies can rigorously interpreted and modeled, and that these discipline-specific topics should be given equal consideration for research support by the ERSD program. That perspective is duly noted in this summary. Suggestions on possible grand-challenge type research topics appropriate for ERSD were also solicited with modest response.

The session opened with a panel discussion on the status of site cleanup at prominent DOE legacy facilities including Hanford, Oak Ridge, Savannah River, and Idaho. The panel discussion was catalyzed by four brief presentations that addressed a series of questions provided to the speakers before the session (**Attachment I**). The speakers were Scott Brooks (ORNL, ERSP_NewOpps_Brooks_ORNL_4_06.pdf); Dan Kaplan (SRS, ERSP_NewOpps_Kaplan_SRS_4_06.pdf); Yoshiko Fujita (INL, ERSP_NewOpps_Fujita_INL_4_06.pdf); and John Zachara (PNNL, ERSP_NewOpps_Zachara_Hanford_4_06.pdf). The four facility information presentations are included as attachments. With the presentation contents as background, the panel discussed: i.) new views on risk-driving DOE contaminants derived from over ten years of active site characterization and restoration, ii.) problematic or vexing environmental fate and transport issues that impede remedial progress, iii.) key gaps in the understanding of contaminant fate and transport and/or *in situ* remediation processes where molecular-level biogeochemical research could make positive contribution, and iv.) translation of biogeochemical research results to the field setting. Several conclusions became evident from the presentations and discussion.

- Remedial pressures are not the same at the four facilities as a result of differences in local regulator and stakeholder competencies, views, values, and expectations.
- Many contaminants will be left in-ground on DOE lands with MNA being the most commonly proposed remedial option.
- Few facility remediation contractors appear to understand the scientific requirements of MNA including the need to identify attenuation processes and quantify attenuation rates.
- Capping to reduce water infiltration is the most commonly used engineered remediation technique on DOE lands, and it is being frequently applied at all four facilities.
- Simplistic models are generally used for performance assessment calculations and the selection of remedial options. Reliance on such calculations may lead to future failures in remedial action performance.

- State of science concepts and models are, in general, not being included in decision-making or remediation activities on DOE lands.
- Microbiologic processes are infrequently considered or included in remedial action evaluations.
- It was not evident that any one of the four facilities was considering the use of bioremediation for the treatment of mobile metals or radioactive constituents in groundwater, in spite of the occurrence of contamination situations that might be amenable to such approach.
- All of the facilities have one or more contaminated sites that present significant challenges for remediation and closure. The contaminant identity and nature of challenge differs between the sites. The knowledge necessary to resolve these challenges does not appear to be current subjects of ERSD research.
- The haste at which cleanup is progressing at DOE sites, and the amount of contaminants being left in ground assures that DOE's legacy waste problems will continue for years after sites have been transferred to long term stewardship.

The facility presentations were followed by a solicitation of research ideas from the session participants that extend NABIR/EMSP research themes to new site needs or science issues. Some participants admitted skepticism as to whether remediation personnel at the facilities have, do, or would avail themselves of new research results given a record that shows little such tendency in the past. Some discussion was had on this perception specifically with regard to whose responsibility it is to assure that the best and most current science and models are used for performance assessment and selection of remedial options. This complex issue is one of many that pervade DOE's cleanup mission and obviously could not be resolved in the breakout session. The session participants were readily able to identify significant extensions of past research themes when the rigorous constraint of direct site applicability was relaxed. These ideas were collected on white-boards, edited for consistency in presentation, and are summarized in **Attachment II** under the categories of *Coupled Processes, Microbiology, Remediation, Biogeochemistry, and Hydrology/Geochemistry*. It should be noted these necessarily represent the perspectives of only those who were at the breakout session, and only those who took the time and effort to respond. Consistent themes that emerged from the participant responses are as follows.

- Greater attention need be given to the rates of in-situ microbiologic and biogeochemical processes under natural conditions as might apply to monitored natural attenuation.
- Process coupling is a critical aspect of engineered remediation schemes, and its impacts should be emphasized for that particular application.
- The nature of process coupling may change at different scales ranging from microscopic to field scales, and research is needed to identify these scale dependencies.
- Mass transfer is a critical determinant of the effectiveness of natural and engineered remediation, and a greater understanding is needed of mass transfer processes at different scales and how they affect subsurface microbiologic and geochemical processes.
- Remedial strategies should be considered that take full advantage of natural processes without stimulation. Stimulated systems may be unstable in the long run, and revert back to original states.
- Since many contaminants may be left in-ground on DOE lands, it is critical to understand immobilization and mobilization processes that may operate during long-term stewardship. Such processes may mitigate or accelerate future potential impacts.

Limited discussion focused on the grand challenge concept. Many did not know the overall goal of the grand challenges, their relationship to other OBER-funded programmatic activities, how they were being financially supported, or how their scope had come to be given the open and competitive nature of OBER funded research. The audience was confused as to the future operational model for the OBER grand challenges, in particular the extent to which they would be tied to the EMSL facility. Perhaps future discussions of grand challenge activities at the ERSP meeting should be well introduced by ERSD Program Staff as to their intent and goals, and questions be fielded to assure complete understanding of the concept by the meeting participants. Some suggested that the full biogeochemical specification of a DOE-relevant aquifer system and the development of a community structure-biogeochemical function model would be a good grand challenge activity for the ERSP. Such an activity has never been accomplished but is now within reach given ERSP research advances. The grand challenge would characterize: phylogeny; interspecies functional and biogeochemical relationships; community structure; hydrophysical relationships; carbon, electron acceptor/donor, and nutrient dynamics; biogeochemical reactions mediated; metabolic and biogeochemical rates; and contaminant biogeochemical dynamics. The research would strive to assemble a linked process/function model of a completely new type and detail level.

Attachment I

NABIR PI Meeting Breakout Session 4: *Identifying New Science Opportunities in Biogeochemistry for DOE Sites*

John Zachara (PNNL) and Eric Roden (University of Wisconsin)

Tuesday, April 4, 2006 ~ 2:15 pm

ABSTRACT

The Environmental Remediation Science Program (ERSP) was established in FY 06 by merging the previous NABIR and EMSP Programs. Coincident with this programmatic change, the Environmental Remediation Sciences Division (ERSD) has been developing a new strategic plan. A draft of the plan is posted on the ERSD website http://www.science.doe.gov/ober/ERSD_top.html. New ideas are sought for the ERSP that extend past NABIR and EMSP research activities on the reductive immobilization of uranium and other polyvalent radionuclides and metals to less explored, but equally relevant and important scientific themes and topics. This breakout session will seek input from ERSP investigators and other meeting participants on new science questions, issues, and opportunities in biogeochemical research for DOE lands. Information is sought on fundamental microbiologic and biogeochemical science topics for fate and transport, stabilization/remediation, natural attenuation, and long term stewardship for DOE risk-driving contaminants. Suggestions on possible grand-challenge type research topics appropriate for ERSD will also be solicited and discussed.

The session will open with a panel discussion on the status of site cleanup at prominent DOE legacy sites including Hanford, Oak Ridge, Savannah River, Los Alamos, and Idaho. The panel will discuss: i.) new views on risk-driving DOE contaminants derived from over ten years of active site characterization and restoration, ii.) problematic or vexing environmental fate and transport issues that impede remedial progress, iii.) key gaps in the understanding of contaminant fate and transport and/or *in situ* remediation processes where molecular-level biogeochemical research could make positive contribution, and iv.) translation of biogeochemical research results to the field setting. These site presentations will be followed by a solicitation of research ideas from the session participants that extend NABIR/EMSP research themes to new site needs or issues. New ideas from the audience will be discussed during the session within the context of the site presentations to identify distinct science themes that will be recorded on different whiteboard panels. All participants will then be asked to circulate around to the different whiteboards and add qualifying or more specific ideas to these themes, or to identify new ones. The participant feedback will then be discussed in open session to identify consensus themes and to prioritize them if possible. The breakout session coordinators will develop a written summary of the proceedings that will be posted on the ERSP website and available for review by all participants one month after the PI meeting.

Tentative Agenda

2:15 - 3:15	Panel discussion on remediation activities and science needs for DOE Sites
3:15 - 4:00	Participant comments and recording of "significant new science opportunities" on whiteboards
4:00 - 4:30	Walk around session for all to add additional ideas to the whiteboards
4:30 - 5:00	Discussion of significant ideas and wrap up

Requests of Panel Members

1. Please describe, in general terms, the major remediation activities that are underway at your site.
2. Who is performing these remedial activities?
3. What are the primary risk driving contaminants that are important at your site?
4. What are the major subsurface contamination problems that your site must deal with in the next 5 years, 10 years, and 20 years?
5. What, in your opinion, are the primary scientific challenges facing restoration and closure of your site?
6. If you had to pick two, visible subsurface contamination problems at your site for which new remedial techniques are critically needed, what would these be?
7. In the years to come, what is your estimate as to the balance between engineered remedial solutions and monitored natural attenuation at your site?
8. In the absence of stimulation, how important are biogeochemical processes in controlling contaminant fate and transport at your site? Which biogeochemical processes, and for which contaminants, are these most significant? Are biogeochemical processes and the subsurface ecology well understood at your site?
9. Are there specific biogeochemical issues associated with long term stewardship at your site?

Attachment I

10. Which biogeochemical processes should be further studied at your site, and how would improved and expanded knowledge assist in decision-making, site cleanup, and long term stewardship?

Attachment II

NOTES: NABIR PI Meeting Breakout Session 4

Research Ideas Contributed by Meeting Participants

Coupled Processes

- Definition: Where a product or outcome is the result of one or more component processes that are functions of the product or outcome.
- Improved modeling – consider all processes, long term.
- More emphasis on microbially-assisted immobilization (indirect vs. direct) – recognizing engineers, stakeholders, regulators preference for more easily controlled processes, and processes that can be implemented in nearer term.
  - ❖ Might the processes still be important even if they don't involve micro-organisms?
  - ❖ Accelerating processes that are already naturally occurring
- Processes coupling at different (multiple) scales. How does the manner of coupling change at different scales.
- Evolving heterogeneity as a result of chemical reaction, microbiologic activity, or geologic facies changes.
- Microscopic reactions and transport controlling long term release rates
- Link between transient fluxes through preferential flow paths and long-term speciation/stability of inorganic contaminants
- Flow ←> Mixing ←> Reactions, e.g. precipitation/dissolution, biofilm formation/decay, phys./chem non-equilibrium
- Illustrating the significance of process coupling in systems that are perturbed at different rates
- Identify and quantify changes to coupled processes resulting from engineered remediation activities
- Relationships between water flow and microbiologic/geochemical processes
  - ❖ Fracture flow
  - ❖ Heterogeneous
  - ❖ Role in long-term performance of "barriers"
- Vadose zone-saturated zone interface: microbial, geochem. & hydrologic processes

Remediation

- Any links between organic and inorganic (metal/radionuclide)_ remediation processes: i.e. for mixed waste
- Effective delivery and in-situ mixing of amendments along a flow path (e.g., phosphate or polyphosphate for U/Sr precipitation). How does one prevent the displacement of the contaminant by the amendment?
- Focus on risk and definition of long-term metrics for remediation (How clean is clean?)
- Fate and transport – health effects
- Natural attenuation
  - ❖ Definition of processes and process succession
  - ❖ Quantification of rates
  - ❖ Modeling
- What is the compelling evidence for/against active/engineered remediation?
- Manipulation (not stimulation) of subsurface microbial ecology (or other processes) to benefit remediation (e.g., reduce cost).
- Remediation/contaminant stabilization in deep vadose zones (e.g. ^{99}Tc at Hanford and ^{90}Sr at INL).

Subsurface Microbiology

- Role of bioengineering (natural enhancement)

Attachment II

- Characterization and retrieval of hard-to-cultivate but environmentally relevant organisms, e.g., in low-energy, low-biomass environments.
- Quantification of rates and activities at low electron donor fluxes.
- Where does microbial activity to occur in deep, variably saturated vadose zones. Does it "bloom" (how fast) and does significant microbial transport occur with rainfall events? Is microbial activity in deep vadose zones significant to long-term contaminant transport.
- Importance of hot spots in microbial activity within narrow physical/chemical gradients at the capillary fringe or groundwater/surface water interface.
- Under what future anticipated (hydrogeochemical) subsurface conditions will microbial activity and growth be stimulated, and to what degree?
- How metabolically diverse and biogeochemically robust are subsurface microbial communities under low recharge conditions?

<u>Biogeochemistry</u>

- Biogeochemical transformations of DOE contaminants under natural/non-stimulated conditions.
    - ❖ carbon or nutrient-limited, long term processes
    - ❖ capacities and rates
- Microbiological influences on contaminant sequestration (Cs, Sr, U, Pu) through biotically-driven, dissolution/reprecipitation and or aqueous complexation reactions.
- Delineating sparse, spatially variable microbiologic communities in oligotrophic environments and identifying their biogeochemical impacts.
- Rates of biogeochemical versus geochemical processes. Identifying regions/zones of predominance and diagnostic markers.

<u>Hydrology/Geochemistry</u>

- Mass transfer processes controlling nutrient, contaminant, and reactant fluxes at different scales.
    - ❖ Intragrain (intragrain fractures and micropores in coatings)
    - ❖ Intrafacies (flow path controlled)
    - ❖ Interfacies (macrostructure control)

<u>Grand Challenge Ideas</u>

- Full biogeochemical specification and function model of a DOE relevant aquifer system.
    - ❖ Phylogeny
    - ❖ Interspecies relationships
    - ❖ Community structure
    - ❖ Hydrogeophysical relationships
    - ❖ Carbon, electron acceptor/donor, and nutrient dynamics
    - ❖ Biogeochemical reactions mediated
    - ❖ Metabolic and biogeochemical rates
    - ❖ Contaminant biogeochemical dynamics.
    - ❖ Linked process model